



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:33 PM UTC

PDB ID : 7WVO / pdb_00007wvo
EMDB ID : EMD-32855
Title : SARS-CoV-2 Omicron S-open-2
Authors : Li, J.W.; Cong, Y.
Deposited on : 2022-02-10
Resolution : 3.41 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

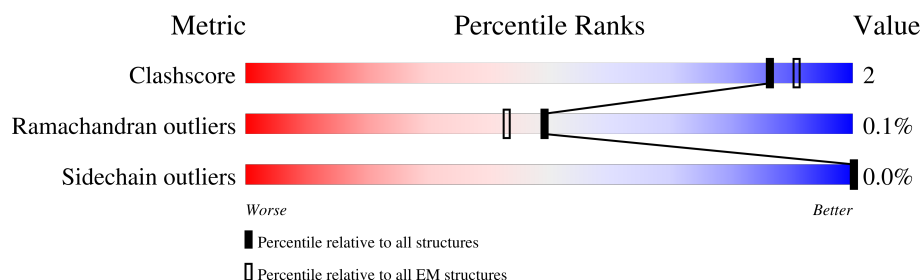
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1258	
1	B	1258	
1	C	1258	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23188 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1048	Total	C	N	O	S	0	0
			8219	5260	1369	1552	38		
1	B	1057	Total	C	N	O	S	0	0
			8293	5307	1382	1566	38		
1	C	856	Total	C	N	O	S	0	0
			6676	4262	1109	1275	30		

There are 303 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	210A	ILE	-	insertion	UNP P0DTC2
A	210B	VAL	-	insertion	UNP P0DTC2
A	210C	ARG	ASN	conflict	UNP P0DTC2
A	210D	GLU	LEU	conflict	UNP P0DTC2
A	210E	PRO	VAL	conflict	UNP P0DTC2
A	210F	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1206	TYR	-	expression tag	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	ASN	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	TYR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	TYR	-	expression tag	UNP P0DTC2
A	1247	LYS	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	ASP	-	expression tag	UNP P0DTC2
A	1251	ASP	-	expression tag	UNP P0DTC2
A	1252	LYS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP P0DTC2
B	210A	ILE	-	insertion	UNP P0DTC2
B	210B	VAL	-	insertion	UNP P0DTC2
B	210C	ARG	ASN	conflict	UNP P0DTC2
B	210D	GLU	LEU	conflict	UNP P0DTC2
B	210E	PRO	VAL	conflict	UNP P0DTC2
B	210F	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1206	TYR	-	expression tag	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	ASN	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	TYR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	TYR	-	expression tag	UNP P0DTC2
B	1247	LYS	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	ASP	-	expression tag	UNP P0DTC2
B	1251	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1252	LYS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	210A	ILE	-	insertion	UNP P0DTC2
C	210B	VAL	-	insertion	UNP P0DTC2
C	210C	ARG	ASN	conflict	UNP P0DTC2
C	210D	GLU	LEU	conflict	UNP P0DTC2
C	210E	PRO	VAL	conflict	UNP P0DTC2
C	210F	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1206	TYR	-	expression tag	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2

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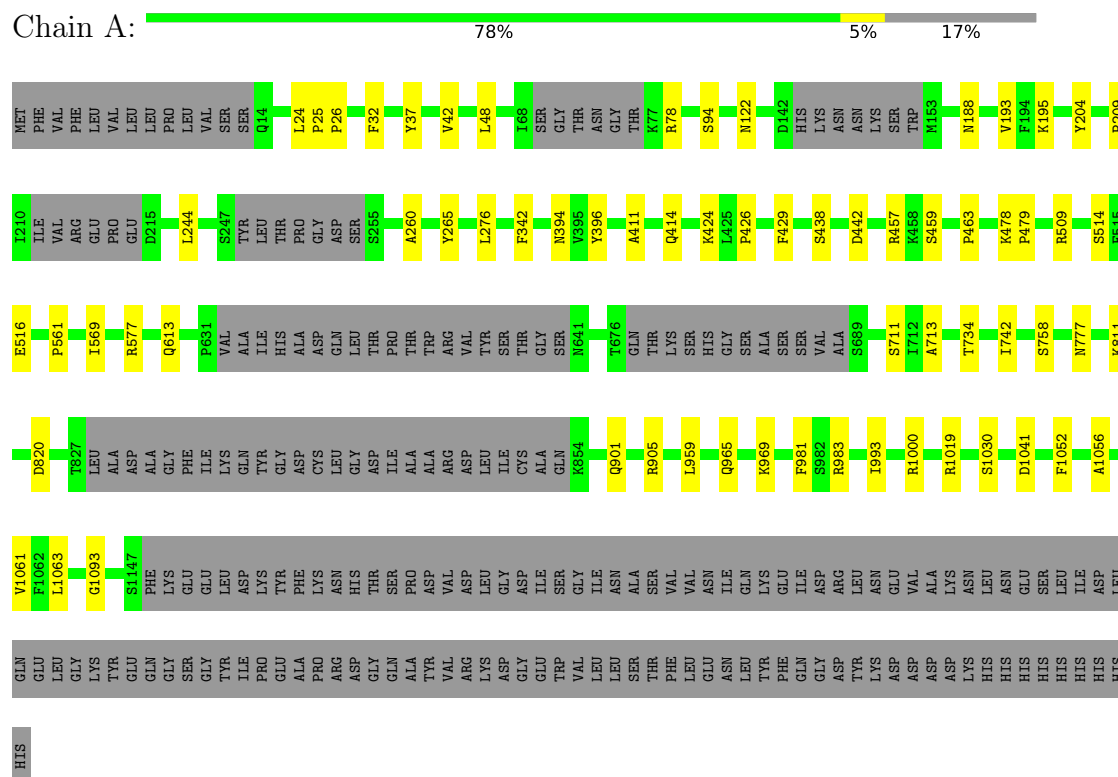
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	ASN	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	TYR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	TYR	-	expression tag	UNP P0DTC2
C	1247	LYS	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	ASP	-	expression tag	UNP P0DTC2
C	1251	ASP	-	expression tag	UNP P0DTC2
C	1252	LYS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2

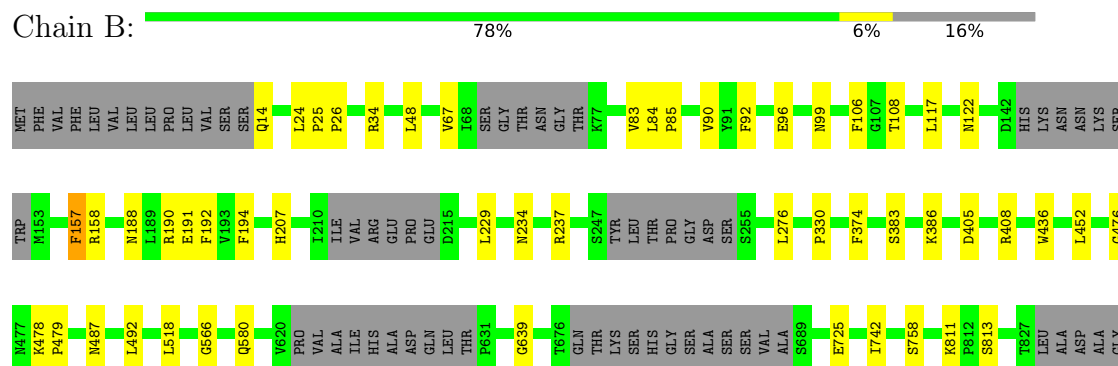
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ARG	ASP	LEU	ILE	CYS	ALA	GLN	K854	G889	M902	N907	Q965	R1000	R1014	E1017	K1028	E1031	L1034	R1039	Y1040	D1041	Y1047	H1048	L1049	F1052	L1063	Y1067	T1077	A1078											
S1147	PHE	LYS	GLU	GLU	LEU	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	LEU	GLY	ASP	ILE	GLY	ASN	ALA	VAL	ASN	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLU	VAL	ALA	LYS	ASN	LEU	ASN	GLU	SER	LEU	ILE	ASP	TRP	GLN	LEU	GLY	TYR

GLU	GLN	SER	PHE	TYR	ILE	PRO	GLU	ALA	GLY	PRO	ASP	ARG	ASN	GLY	GLN	TYR	VAL	ARG	LYS	ASP	GLY	GLY	TRP	VAL	LEU	GLU	ASN	GLN	PHE	GLY	ASP	LYS	ASN	ASP	ASP	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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● Molecule 1: Spike glycoprotein



MET	PHE	VAL	LEU	VAL	LEU	LEU	PRO	GLY	LEU	VAL	SER	Q114	R21	R34	H66	V67	I68	SER	GLY	THR	ASN	THR	K77	R78	N81	E96	R102	F106	G107	T108	L117	M122	D142	LYS	ASN	ASN	LYS	TRP	M153	E156	F157	R190	E191
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I203	K206	I210	ILE	VAL	ARG	GLY	PRO	GLY	D215	Q218	L223	L226	V227	N234	S247	TYR	LEU	THR	PRO	GLY	ASP	SER	S255	L276	C301	N317	E324	R328	PHE	PRO	ASN	ILE	THR	ASN	LEU	VAL	CYS	PRO	PHE	ASP	GLU	VAL	PHE	ASN	ALA	THR	ARG
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PHE	ALA	VAL	TYR	TRP	ASN	ARG	LYS	GLY	ILE	ASN	SER	ASN	CYS	VAL	ALA	ASP	TYR	LEU	ALA	PHE	PHE	THR	PHE	LYS	CYS	TYR	GLY	VAL	PRO	THR	LYS	LEU	ASN	ASP	CYS	PHE	THR	ASN	VAL	VAL	ARG	THR	ILE	ARG	GLY	ASP	GLU
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VAL	ARG	GLN	ILE	ALA	PRO	GLY	GLN	THR	GLY	ASN	ASP	ASP	ASP	PHE	THR	GLY	CYS	VAL	ILE	ALA	TRP	THR	ASN	SER	ASN	LYS	VAL	SER	GLY	VAL	SER	GLY	ASN	TYR	ASN	TYR	LEU	TYR	THR	ARG	LEU	PHE	ASN	LEU	LYS	PRO	PHE	THR	ARG
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ASP	ILE	SER	THR	GLU	ILE	TYR	GLN	ALA	GLY	PRO	CYS	ASN	GLY	VAL	ALA	GLY	PHE	ASN	CYS	THR	PHE	PRO	LEU	ARG	THR	LYS	GLY	VAL	GLY	HIS	GLY	PRO	GLN	SER	TYR	ARG	VAL	VAL	VAL	LEU	SER	PHE	GLU	LEU	LEU	ALA	ALA	PRO	ALA	THR	VAL	CYS	GLY
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PRO	LYS	S530	V539	P561	R577	G594	V620	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU	THR	P631	G639	C671	A672	T676	GLN	THR	LYS	SER	HIS	GLY	SER	ALA	SER	VAL	ALA	S889	I742	C743	G744	Q755	S758	T827	LEU	ALA	ASP	ALA	ALA	GLY
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PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	ALA	ALA	ARG	ASP	GLY	LEU	ILE	CYS	ALA	K854	F855	K856	L861	Q895	A903	Y904	Q913	Q965	L977	R1000	R1014	E1017	S1030	Y1047	F1052	L1063	Y1067	R1107	S1147	PHE	LYS	GLU
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GLU	LEU	ASP	LYS	PHE	PHE	LYS	ASN	ASN	THR	PRO	VAL	VAL	ASP	GLY	ILE	SER	GLY	ILE	ASN	VAL	VAL	ASN	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLU	VAL	SER	LEU	ILE	ASP	GLN	GLU	LEU	GLY	LYS	TYR	GLU	GLN	GLY	SER
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GLY	TYR	PRO	GLU	ALA	PRO	ARG	ASP	GLY	GLN	ALA	TYR	VAL	VAL	ASP	GLY	TRP	VAL	GLY	ILE	ASN	THR	SER	THR	PHE	LEU	GLU	ASN	GLY	ASP	TYR	LYS	ASN	GLU	VAL	ASP	ASP	ASP	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38906	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/8410	0.52	2/11435 (0.0%)
1	B	0.28	0/8487	0.54	6/11540 (0.1%)
1	C	0.27	0/6819	0.52	4/9267 (0.0%)
All	All	0.28	0/23716	0.53	12/32242 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	PHE	CA-C-N	6.50	133.40	121.70
1	B	157	PHE	C-N-CA	6.50	133.40	121.70
1	B	122	ASN	CA-C-N	6.12	133.23	121.54
1	B	122	ASN	C-N-CA	6.12	133.23	121.54
1	A	122	ASN	CA-C-N	5.97	132.95	121.54
1	A	122	ASN	C-N-CA	5.97	132.95	121.54
1	C	639	GLY	CA-C-N	5.57	132.18	121.54
1	C	639	GLY	C-N-CA	5.57	132.18	121.54
1	B	639	GLY	CA-C-N	5.45	131.95	121.54
1	B	639	GLY	C-N-CA	5.45	131.95	121.54
1	C	156	GLU	CA-C-N	5.33	131.29	121.70
1	C	156	GLU	C-N-CA	5.33	131.29	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	PHE	Peptide
1	C	157	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8219	0	8052	39	0
1	B	8293	0	8121	37	0
1	C	6676	0	6566	32	0
All	All	23188	0	22739	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HB3	1:A:25:PRO:HD2	1.64	0.80
1:B:24:LEU:HB3	1:B:25:PRO:HD2	1.79	0.63
1:A:24:LEU:HD21	1:A:78:ARG:HD2	1.85	0.59
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.88	0.56
1:A:48:LEU:HD11	1:A:276:LEU:HB3	1.89	0.55
1:A:569:ILE:HG13	1:C:856:LYS:HZ1	1.73	0.54
1:C:21:ARG:HH22	1:C:81:ASN:HB3	1.72	0.54
1:B:1052:PHE:HB2	1:B:1063:LEU:HB2	1.90	0.53
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.92	0.52
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.90	0.52
1:A:758:SER:OG	1:B:965:GLN:NE2	2.43	0.51
1:A:24:LEU:HB3	1:A:25:PRO:CD	2.38	0.50
1:A:438:SER:HB3	1:A:442:ASP:HB2	1.93	0.50
1:A:983:ARG:HH22	1:B:518:LEU:HD11	1.77	0.50
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.93	0.50
1:B:811:LYS:HE2	1:B:813:SER:HB3	1.94	0.50
1:A:1030:SER:HB2	1:B:1041:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:HB	1:B:194:PHE:HB2	1.94	0.49
1:A:613:GLN:HE22	1:C:861:LEU:HD23	1.77	0.49
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.45	0.49
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.45	0.49
1:A:342:PHE:O	1:A:509:ARG:NH1	2.45	0.49
1:B:83:VAL:HG12	1:B:237:ARG:HD3	1.95	0.49
1:C:324:GLU:H	1:C:539:VAL:HG12	1.78	0.49
1:B:374:PHE:HA	1:B:436:TRP:HD1	1.79	0.48
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.46	0.48
1:C:561:PRO:O	1:C:577:ARG:NH1	2.47	0.48
1:A:965:GLN:NE2	1:C:758:SER:OG	2.46	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HB2	1.96	0.47
1:C:96:GLU:OE1	1:C:190:ARG:NH2	2.48	0.47
1:A:394:ASN:HB2	1:A:516:GLU:HB3	1.95	0.47
1:B:96:GLU:OE1	1:B:190:ARG:NH2	2.48	0.47
1:A:561:PRO:O	1:A:577:ARG:NH1	2.48	0.46
1:B:405:ASP:O	1:B:408:ARG:NH1	2.48	0.46
1:B:99:ASN:OD1	1:B:190:ARG:NH2	2.50	0.45
1:C:276:LEU:HD11	1:C:301:CYS:HA	1.99	0.45
1:C:203:ILE:HD12	1:C:227:VAL:HB	1.99	0.45
1:A:713:ALA:HB3	1:C:895:GLN:H	1.81	0.45
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.50	0.45
1:C:108:THR:OG1	1:C:234:ASN:O	2.35	0.45
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.99	0.44
1:A:42:VAL:HG13	1:B:566:GLY:HA2	1.99	0.44
1:C:744:GLY:H	1:C:977:LEU:HD12	1.81	0.44
1:A:981:PHE:HB2	1:A:993:ILE:HD11	1.99	0.44
1:B:14:GLN:O	1:B:158:ARG:NH1	2.44	0.44
1:C:66:HIS:HD2	1:C:78:ARG:HE	1.65	0.44
1:C:34:ARG:NH2	1:C:218:GLN:O	2.46	0.44
1:B:188:ASN:OD1	1:B:207:HIS:NE2	2.49	0.44
1:A:1041:ASP:HB2	1:C:1030:SER:HB2	2.00	0.43
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.51	0.43
1:A:457:ARG:NH1	1:A:459:SER:OG	2.50	0.43
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.48	0.43
1:B:758:SER:OG	1:C:965:GLN:NE2	2.49	0.43
1:C:1014:ARG:NH1	1:C:1017:GLU:OE1	2.52	0.43
1:A:424:LYS:HG3	1:A:463:PRO:HG3	2.01	0.43
1:B:229:LEU:H	1:B:229:LEU:HG	1.68	0.43
1:B:476:GLY:H	1:B:487:ASN:HB3	1.83	0.43
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PRO:HG2	1:A:429:PHE:HB2	2.01	0.43
1:B:889:GLY:HA3	1:B:1034:LEU:HD22	2.01	0.43
1:B:108:THR:OG1	1:B:234:ASN:O	2.37	0.42
1:B:383:SER:HB3	1:B:386:LYS:HB2	2.02	0.42
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.53	0.42
1:A:711:SER:OG	1:C:895:GLN:NE2	2.52	0.42
1:B:48:LEU:HB3	1:B:276:LEU:HD11	2.01	0.42
1:B:106:PHE:HB2	1:B:117:LEU:HB3	2.02	0.42
1:B:330:PRO:HA	1:B:580:GLN:HG2	2.00	0.42
1:B:84:LEU:HA	1:B:85:PRO:HD3	1.86	0.42
1:C:206:LYS:HB2	1:C:223:LEU:HA	2.01	0.42
1:B:902:MET:HE1	1:B:1049:LEU:HD13	2.01	0.41
1:C:903:ALA:HB1	1:C:913:GLN:HG2	2.02	0.41
1:A:193:VAL:HB	1:A:204:TYR:HB2	2.02	0.41
1:A:777:ASN:HD21	1:A:1019:ARG:HG2	1.86	0.41
1:A:734:THR:HG21	1:A:959:LEU:HD21	2.01	0.41
1:A:901:GLN:HB3	1:A:905:ARG:HH12	1.84	0.41
1:B:1014:ARG:NH1	1:B:1017:GLU:OE1	2.53	0.41
1:C:671:CYS:SG	1:C:672:ALA:N	2.93	0.41
1:A:969:LYS:HD2	1:C:755:GLN:HG2	2.03	0.41
1:A:244:LEU:HG	1:A:260:ALA:HB2	2.01	0.41
1:B:452:LEU:HD13	1:B:492:LEU:HD21	2.02	0.41
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.03	0.41
1:B:478:LYS:HD2	1:B:479:PRO:HD2	2.03	0.41
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.02	0.41
1:A:1056:ALA:HB2	1:A:1061:VAL:HG23	2.03	0.40
1:B:907:ASN:HD22	1:C:1107:ARG:HH22	1.68	0.40
1:B:1031:GLU:OE1	1:B:1039:ARG:NH1	2.54	0.40
1:A:94:SER:HA	1:A:265:TYR:HA	2.04	0.40
1:A:188:ASN:HA	1:A:209:PRO:HA	2.03	0.40
1:A:478:LYS:HD2	1:A:479:PRO:HD2	2.03	0.40
1:B:92:PHE:HB3	1:B:192:PHE:HB2	2.03	0.40
1:A:1093:GLY:O	1:C:904:TYR:OH	2.37	0.40
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.54	0.40
1:C:102:ARG:HH21	1:C:122:ASN:HA	1.85	0.40
1:C:317:ASN:HA	1:C:594:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1032/1258 (82%)	987 (96%)	43 (4%)	2 (0%)	43	71
1	B	1041/1258 (83%)	1002 (96%)	38 (4%)	1 (0%)	48	78
1	C	838/1258 (67%)	810 (97%)	28 (3%)	0	100	100
All	All	2911/3774 (77%)	2799 (96%)	109 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	PRO
1	A	32	PHE
1	A	26	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	765/1099 (70%)	765 (100%)	0	100	100
1	B	705/1099 (64%)	704 (100%)	1 (0%)	88	88
1	C	750/1099 (68%)	750 (100%)	0	100	100
All	All	2220/3297 (67%)	2219 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	164	ASN
1	A	188	ASN
1	A	196	ASN
1	A	271	GLN
1	A	414	GLN
1	A	505	HIS
1	A	540	ASN
1	A	613	GLN
1	A	777	ASN
1	A	913	GLN
1	A	914	ASN
1	A	965	GLN
1	B	49	HIS
1	B	61	ASN
1	B	409	GLN
1	B	437	ASN
1	B	542	ASN
1	B	564	GLN
1	B	644	GLN
1	B	717	ASN
1	B	787	GLN
1	B	907	ASN
1	B	913	GLN
1	B	965	GLN
1	B	992	GLN
1	B	1064	HIS
1	B	1083	HIS
1	B	1088	HIS
1	C	14	GLN
1	C	30	ASN
1	C	66	HIS
1	C	134	GLN
1	C	196	ASN
1	C	239	GLN
1	C	271	GLN
1	C	542	ASN
1	C	564	GLN

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Mol	Chain	Res	Type
1	C	717	ASN
1	C	895	GLN
1	C	914	ASN
1	C	965	GLN
1	C	1002	GLN
1	C	1108	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32855. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.